

Effective Equations for the Precession Dynamics of Electron Spins and Electron-Impurity Correlations in Diluted Magnetic Semiconductors

M. Cygorek, V. M. Axt

Theoretische Physik III, Universität Bayreuth, 95440 Bayreuth, Germany

Abstract. Starting from a quantum kinetic theory for the spin dynamics in diluted magnetic semiconductors, we derive simplified equations that effectively describe the spin transfer between carriers and magnetic impurities for an arbitrary initial impurity magnetization. Taking the Markov limit of these effective equations, we obtain good quantitative agreement with the full quantum kinetic theory for the spin dynamics in bulk systems at high magnetic doping. In contrast, the standard rate description where the carrier-dopant interaction is treated according to Fermi's golden rule, which involves the assumption of a short memory as well as a perturbative argument, has been shown previously to fail if the impurity magnetization is non-zero. The Markov limit of the effective equations is derived, assuming only a short memory, while higher order terms are still accounted for. These higher order terms represent the precession of the carrier-dopant correlations in the effective magnetic field due to the impurity spins. Numerical calculations show that the Markov limit of our effective equations reproduces the results of the full quantum kinetic theory very well. Furthermore, this limit allows for analytical solutions and for a physically transparent interpretation.

PACS numbers: 75.78.Jp, 75.50.Pp, 75.30.Hx, 72.10.Fk

1. Introduction

Diluted magnetic semiconductors (DMS), in particular Mn doped II-VI and III-V materials, have been studied for several decades[1–18]. However, the theoretical description of the ultrafast spin dynamics of the magnetic impurities and carriers is, so far, mostly limited to a single-particle mean-field picture, where transfer rates are calculated perturbatively by Fermi’s golden rule. Interesting features of the spin dynamics in DMS that have been demonstrated in recent time-resolved Kerr measurements[19], like the nonmonotonous dependence of the transverse spin dephasing time in extremely diluted $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ quantum wells or the mismatch between the theoretically predicted and experimentally measured dephasing times for zero magnetic field, still lack a satisfactory theoretical explanation. To provide a more elaborate theoretical framework for the discussion and quantitative calculation of the spin dynamics in DMS, a quantum kinetic theory based on a correlation expansion has been introduced[20] where the exchange interaction between free carriers and the d electrons of the Mn impurities was modelled by a Kondo Hamiltonian. The full quantum kinetic theory is, however, numerically challenging and the physical interpretation requires some effort. Hence, it is a difficult task to efficiently implement other mechanisms of spin exchange and dephasing into the theory in order to account for effects that are in many cases needed for a proper description of real experiments like, e. g., the D’yakonov-Perel’[21], Elliot-Yafet[22, 23] and Bir-Aronov-Pikus[24] mechanisms. However, it was already shown that for three dimensional systems in which the number of Mn impurities N_{Mn} exceeds the number of free carriers N_e , a simplification of the quantum kinetic theory can be established that reasonably reproduces results in the case of a vanishing initial Mn magnetization[25]. This was achieved by a perturbative treatment of the carrier-impurity interaction as well as the assumption of a short memory. This procedure yielded the same rate equations as Fermi’s golden rule. In contrast, for a nonzero average Mn spin these rate equations were shown to describe only the electron spin component perpendicular to the Mn spin well, while a discrepancy in the dynamics of the parallel electron spin component could be attributed to neglected terms of higher than leading order in the coupling constant J_{sd} of the Kondo Hamiltonian (1) in the perturbative derivation of the rate equations in Ref. [26].

In the present article, we derive approximate equations of motion for the electron spins in the spirit of the equations in Ref. [26], but take the higher order corrections into account. These equations describe the effects of the precession of the electron spins around the effective magnetic field due to the Mn magnetization and effectively account for a precession-type dynamics of the electron-Mn correlations that has been identified previously in Ref. [26]. The resulting *precession of electron spins and correlations* (PESC) equations are then discussed and their Markov limit is established which can be solved analytically. Numerical calculations show that for $N_{Mn} \gg N_e$ these analytical solutions coincide with the results of the full quantum kinetic theory, at least in three dimensional systems. The simplicity of the PESC equations makes it possible to easily interpret the basic physical processes involved in the quantum kinetic theory and allows the PESC equations to provide a suitable framework for further studies of non-Markovian effects as well as of the interplay between the s - d interaction and other mechanisms of spin relaxation and dephasing.

It is noteworthy that the derived effective equations are expected to be applicable not only for the spin dynamics in DMS, but they can easily be extended to describe

more generally any system, in which a continuum of states is coupled to localized magnetic impurities via a Kondo-like Hamiltonian

$$H = \sum_{l\mathbf{k}} E_{\mathbf{k}} c_{l\mathbf{k}}^\dagger c_{l\mathbf{k}} + J_{sd} \sum_{Ii} \hat{\mathbf{S}}^I \cdot \hat{\mathbf{s}}^i \delta(\mathbf{R}_I - \mathbf{r}_i), \quad (1)$$

where in the case of DMS $c_{l\mathbf{k}}^\dagger$ and $c_{l\mathbf{k}}$ describe creation and annihilation operators for conduction band electrons with wave vector \mathbf{k} in the subband l , $E_{\mathbf{k}}$ are the corresponding single-particle energies, $\hat{\mathbf{S}}^I$ and $\hat{\mathbf{s}}^i$ are the spin operators while \mathbf{R}_I and \mathbf{r}_i are the positions of the I -th Mn ion and the i -th electron, respectively. Similar magnetic interactions can also arise from nuclear spins due to the Fermi contact interaction or an effective interaction between conduction band electrons and localized states, such as in quantum dots, or quasi-particles, e. g. excitons, in a huge variety of systems ranging from semiconductor heterostructures to novel materials such as graphene or dichalcogenides, since the main difference between these systems lies in the details of the single-particle band structures. Therefore, the equations of motion studied here are of prototypical character for the spin dynamics of extended systems.

The article is outlined as follows: First, we summarize the quantum kinetic theory and reproduce the basic equations of motion where we restrict ourselves to the terms that were shown in Ref. [26] to be numerically important in the case $N_{Mn} \gg N_e$. In a next step, we apply a rotating-wave-like approximation and derive the PESC equations of motion for the electron spins and occupations. Then, the Markov limit of the PESC equations is introduced, and the thereby described physical effects are discussed; in particular the spectral redistribution of electrons as well as Pauli blocking effects are shown to arise naturally on this level of theory. Subsequently, analytical solutions to the Markov limit of the PESC equations are presented and compared with numerical results of the full quantum kinetic theory.

2. Method: Derivation of Effective Equations

We will give a short overview of the quantum kinetic theory for the spin dynamics in DMS developed in Ref. [20]. There, a systematic derivation of equations of motion for the spins of interacting carriers and Mn impurities in DMS has been presented accounting for conduction and valence band carriers, their coherences, the Mn impurity spins, the correlations between carriers and impurities as well as the effect of an external laser field, where a disorder average over the random distribution of the impurities in the semiconductor was performed. Apart from the corresponding band energies, the theory accounts for the exchange interaction between carriers and Mn impurities as well as for the dipole coupling to a classical laser field.

We want to focus our study on the spin dynamics in isoelectrically doped bulk DMS starting from a non-equilibrium state. Such kind of situation can be prepared, e.g., by optical excitation with circularly polarized light. Since in bulk systems, the typical timescale of the hole spin relaxation is of the order of 100 fs [27] due to the strong spin-orbit interaction, we can neglect the valence band and the interband coherences when concentrating on a ps timescale. When only the conduction band electrons and the impurities together with their correlations are considered, the resulting equations of motion can be simplified as it was shown in Ref. [26]. The dynamical variables used in this subset of equations are the conduction band electron density matrices $C_{l_1\mathbf{k}_1}^{l_2}$, the average Mn density matrix $M_{n_1}^{n_2}$ and their correlations $Q_{l_1n_1\mathbf{k}_1}^{l_2n_2\mathbf{k}_2}$:

$$C_{l_1\mathbf{k}_1}^{l_2} = \langle c_{l_1\mathbf{k}_1}^\dagger c_{l_2\mathbf{k}_1} \rangle, \quad (2a)$$

$$M_{n_1}^{n_2} = \langle \hat{P}_{n_1 n_2}^I \rangle, \quad (2b)$$

$$Q_{l_1 n_1 \mathbf{k}_1}^{l_2 n_2 \mathbf{k}_2} = \delta \langle c_{l_1 \mathbf{k}_1}^\dagger c_{l_2 \mathbf{k}_2} \hat{P}_{n_1 n_2}^I e^{i(\mathbf{k}_2 - \mathbf{k}_1) \mathbf{R}_I} \rangle \\ + \delta \langle c_{l_1 \mathbf{k}_1}^\dagger c_{l_2 \mathbf{k}_2} e^{i(\mathbf{k}_2 - \mathbf{k}_1) \mathbf{R}_I} \rangle \langle \hat{P}_{n_1 n_2}^I \rangle, \quad (2c)$$

where $c_{l_1 \mathbf{k}_1}^\dagger$ and $c_{l_1 \mathbf{k}_1}$ are the electron creation and annihilation operators, $\hat{P}_{n_1 n_2}^I = |I, n_1\rangle \langle I, n_2|$ is the density operator for the spin- $\frac{5}{2}$ state of the d electrons of the I -th Mn ion, and the indices $l_i \in \{1, 2\}$ as well as $n_i \in \{-\frac{5}{2}, -\frac{3}{2}, \dots, \frac{5}{2}\}$ represent spin indices of the conduction band electrons and Mn spin states, respectively. The brackets symbolize the quantum mechanical average as well as the disorder average over the random distribution of the Mn positions \mathbf{R}_I and $\delta \langle \dots \rangle$ describes the true correlations, i. e., the average value minus all possible factorized parts (cf. Refs. [20] for the details of the correlation expansion and the truncation scheme).

In Ref. [26] it was also found that considering only the numerically important terms, the correlations can be summed up together with the electron and Mn spin matrices yielding new correlation functions with fewer degrees of freedom:

$$Q_{\beta \mathbf{k}_1}^{\alpha \mathbf{k}_2} := \sum_{\substack{l_1 l_2 \\ n_1 n_2}} S_{n_1 n_2}^\beta s_{l_1 l_2}^\alpha Q_{l_1 n_1 \mathbf{k}_1}^{l_2 n_2 \mathbf{k}_2}, \quad (3)$$

where $s_{l_1 l_2}^\alpha$ with $\alpha \in \{0, 1, 2, 3\}$ are the electron spin matrices and the identity matrix (for $\alpha = 0$), respectively, and S^β with $\beta \in \{1, 2, 3\}$ are the spin- $\frac{5}{2}$ matrices for the Mn ions. The equations of motion for the electron occupations $n_{\mathbf{k}_1} = \sum_l C_{l \mathbf{k}_1}^l$ and spins $s_{\mathbf{k}_1}^\alpha = \sum_{ll'} s_{ll'}^\alpha C_{l \mathbf{k}_1}^{l'}$ are then given by [20, 26]:

$$\frac{\partial}{\partial t} n_{\mathbf{k}_1} = \frac{J_{sd}}{\hbar} n_{Mn} \frac{1}{V} \sum_{\mathbf{k}} \sum_{i=1}^3 2\Im(Q_{i \mathbf{k}_1}^i), \quad (4a)$$

$$\frac{\partial}{\partial t} s_{\mathbf{k}_1}^\alpha = \frac{J_{sd}}{\hbar} n_{Mn} \left\{ (\langle \mathbf{S} \rangle \times \mathbf{s}_{\mathbf{k}_1})_\alpha + \right. \\ \left. + \frac{1}{V} \sum_{\mathbf{k}} \left[\frac{1}{2} \Im(Q_{\alpha \mathbf{k}_1}^{0 \mathbf{k}}) + \sum_{ij=1}^3 \epsilon_{ij\alpha} \Re(Q_{i \mathbf{k}_1}^{j \mathbf{k}}) \right] \right\}, \quad (4b)$$

$$\frac{\partial}{\partial t} Q_{\beta \mathbf{k}_1}^{\alpha \mathbf{k}_2} = -i(\omega_{\mathbf{k}_2} - \omega_{\mathbf{k}_1}) Q_{\beta \mathbf{k}_1}^{\alpha \mathbf{k}_2} + \\ + \frac{i}{\hbar} J_{sd} \left(b_{\beta \mathbf{k}_1}^{\alpha \mathbf{k}_2 I.1} + b_{\beta \mathbf{k}_1}^{\alpha \mathbf{k}_2 I.2} + b_{\beta \mathbf{k}_1}^{\alpha \mathbf{k}_2 II.1} + b_{\beta \mathbf{k}_1}^{\alpha \mathbf{k}_2 Res} \right), \quad (4c)$$

with source terms

$$b_{\beta \mathbf{k}_1}^{\alpha \mathbf{k}_2 I.1} = \sum_{\gamma} \sum_{l_1 l_2} \left(\langle S^\gamma S^\beta \rangle s_{l_1}^\gamma s_{l_1 l_2}^\alpha C_{l \mathbf{k}_2}^{l_2} - \langle S^\beta S^\gamma \rangle s_{l_1 l_2}^\alpha s_{l_2 l}^\gamma C_{l_1 \mathbf{k}_1}^l \right), \quad (4d)$$

$$b_{\beta \mathbf{k}_1}^{\alpha \mathbf{k}_2 I.2} = -i \sum_{\gamma \delta} \epsilon_{\gamma \beta \delta} \sum_{ll' l_1 l_2} \langle S^\delta \rangle \{ s_{ll'}^\gamma C_{l_1 \mathbf{k}_1}^{l'} s_{l_1 l_2}^\alpha C_{l \mathbf{k}_2}^{l_2} \}, \quad (4e)$$

$$b_{\beta \mathbf{k}_1}^{\alpha \mathbf{k}_2 II.1} = i \sum_{\gamma \delta} \epsilon_{\gamma \alpha \delta} n_{Mn} \langle S^\gamma \rangle Q_{\beta \mathbf{k}_1}^{\delta \mathbf{k}_2} = -i \frac{\hbar}{J_{sd}} (\boldsymbol{\omega}_M \times \mathbf{Q}_{\beta \mathbf{k}_1}^{\mathbf{k}_2})_\alpha, \quad (4f)$$

where $\langle S^\alpha \rangle = \sum_{n_1 n_2} S_{n_1 n_2}^\alpha M_{n_1}^{n_2}$ are the averages of the Mn spin operators and $\langle S^\alpha S^\beta \rangle = \sum_{n_1 n_2 n} S_{n_1 n}^\alpha S_{nn_2}^\beta M_{n_1}^{n_2}$ its second moments. V represents the volume of the sample, $n_{Mn} = \frac{N_{Mn}}{V}$ is the Mn density and the \mathbf{k} -sum has to be performed over all states

in the first Brillouin zone. $b_{\beta\mathbf{k}_1}^{\alpha\mathbf{k}_2 Res}$ comprise the residual source terms that were identified in Ref. [26] to be insignificant if $N_{Mn} \gg N_e$ and V is large. Therefore, we will henceforth neglect $b_{\beta\mathbf{k}_1}^{\alpha\mathbf{k}_2 Res}$.

In Eq. (4f), the mean field precession frequency and axis of the electrons around the Mn magnetization $\omega_M := \frac{J_{sd}}{\hbar} n_{Mn} \langle \mathbf{S} \rangle$ has been introduced as well as the vector representation of the correlations $(\mathbf{Q}_{\beta\mathbf{k}_1}^{\mathbf{k}_2})_\alpha := Q_{\beta\mathbf{k}_1}^{\alpha\mathbf{k}_2}$. $\omega_{\mathbf{k}} = \frac{E_{\mathbf{k}}}{\hbar} = \frac{\hbar\mathbf{k}^2}{2m^*}$ describes the single-particle frequencies of the quasi-free conduction band electrons assuming a parabolic band structure with effective mass m^* without the electron-Mn exchange interaction. $b_{\beta\mathbf{k}_1}^{\alpha\mathbf{k}_2 I.1}$ is the source term describing the build-up of correlations between the impurities and the carriers, while $b_{\beta\mathbf{k}_1}^{\alpha\mathbf{k}_2 I.2}$ provides corrections to $b_{\beta\mathbf{k}_1}^{\alpha\mathbf{k}_2 I.1}$ due to (mean field) two-electron effects, e. g., Pauli blocking[26]. The precession-type dynamics of the carrier-Mn correlations around the effective magnetic field due to the Mn magnetization are incorporated via the term $b_{\beta\mathbf{k}_1}^{\alpha\mathbf{k}_2 II.1}$. The neglect of the latter has been found to be the reason for the failure of the golden rule-type rate equations of Ref. [26] in describing the parallel spin transfer between the carriers and the magnetic impurities.

It is, however, possible to account for this precession and to integrate Eq. (4c) formally. This is particularly easy if we use the assumption $N_{Mn} \gg N_e$ that allows us to regard the Mn density matrix as nearly constant in time. If the z-axis is defined to point in the direction of the Mn magnetization, the correlations are given by:

$$Q_{\beta\mathbf{k}_1}^{0\mathbf{k}_2} = \frac{i}{\hbar} J_{sd} \int_0^t dt' \left\{ b_{\beta\mathbf{k}_1}^{0\mathbf{k}_2 I}(t') e^{i(\omega_{\mathbf{k}_2} - \omega_{\mathbf{k}_1})(t' - t)} \right\}, \quad (5a)$$

$$Q_{\beta\mathbf{k}_1}^{x\mathbf{k}_2} = \frac{i}{2\hbar} J_{sd} \int_0^t dt' \left\{ (b_{\beta\mathbf{k}_1}^{x\mathbf{k}_2 I}(t') + i b_{\beta\mathbf{k}_1}^{y\mathbf{k}_2 I}(t')) e^{i(\omega_{\mathbf{k}_2} - \omega_{\mathbf{k}_1} - \omega_M)(t' - t)} + (b_{\beta\mathbf{k}_1}^{x\mathbf{k}_2 I}(t') - i b_{\beta\mathbf{k}_1}^{y\mathbf{k}_2 I}(t')) e^{i(\omega_{\mathbf{k}_2} - \omega_{\mathbf{k}_1} + \omega_M)(t' - t)} \right\} \quad (5b)$$

$$Q_{\beta\mathbf{k}_1}^{y\mathbf{k}_2} = \frac{i}{2\hbar} J_{sd} \int_0^t dt' \left\{ (b_{\beta\mathbf{k}_1}^{y\mathbf{k}_2 I}(t') - i b_{\beta\mathbf{k}_1}^{x\mathbf{k}_2 I}(t')) e^{i(\omega_{\mathbf{k}_2} - \omega_{\mathbf{k}_1} - \omega_M)(t' - t)} + (b_{\beta\mathbf{k}_1}^{y\mathbf{k}_2 I}(t') + i b_{\beta\mathbf{k}_1}^{x\mathbf{k}_2 I}(t')) e^{i(\omega_{\mathbf{k}_2} - \omega_{\mathbf{k}_1} + \omega_M)(t' - t)} \right\} \quad (5c)$$

$$Q_{\beta\mathbf{k}_1}^{z\mathbf{k}_2} = \frac{i}{\hbar} J_{sd} \int_0^t dt' \left\{ b_{\beta\mathbf{k}_1}^{z\mathbf{k}_2 I}(t') e^{i(\omega_{\mathbf{k}_2} - \omega_{\mathbf{k}_1})(t' - t)} \right\} \quad (5d)$$

where $b_{\beta\mathbf{k}_1}^{\alpha\mathbf{k}_2 I} := b_{\beta\mathbf{k}_1}^{\alpha\mathbf{k}_2 I.1} + b_{\beta\mathbf{k}_1}^{\alpha\mathbf{k}_2 I.2}$. In order to simplify Eqs. (5), we follow the line of Ref. [26] and identify fast and slowly changing terms. To this end, we express the electron spin in the state with k-vector \mathbf{k}_1

$$\mathbf{s}_{\mathbf{k}_1} := \begin{pmatrix} s_{\mathbf{k}_1}^\perp \cos(\omega_M t + \varphi_{\mathbf{k}_1}) \\ s_{\mathbf{k}_1}^\perp \sin(\omega_M t + \varphi_{\mathbf{k}_1}) \\ s_{\mathbf{k}_1}^\parallel \end{pmatrix}, \quad (6)$$

in terms of the spin component parallel to the Mn magnetization $s_{\mathbf{k}_1}^\parallel$, the perpendicular spin component $s_{\mathbf{k}_1}^\perp$ and the phase $\varphi_{\mathbf{k}_1}$. A rotating-wave-like approximation is

established, by assuming that these variables $s_{\mathbf{k}_1}^{\parallel}, s_{\mathbf{k}_1}^{\perp}$ and $\varphi_{\mathbf{k}_1}$ as well as the electron occupation $n_{\mathbf{k}_1}$ of the states with \mathbf{k} -vector \mathbf{k}_1 change only slowly in time, since they are constant in the mean field approximation. When they are drawn out of the integrals in Eqs. (5) and the resulting expressions for the correlations are inserted in the equations of motion (4a) and (4b) for the electron occupations and spins, we get:

$$\begin{aligned} \frac{\partial}{\partial t} n_{\mathbf{k}_1}^{\uparrow/\downarrow} = \sum_{\mathbf{k}} \left\{ \Re(G_{\omega_{\mathbf{k}}}^{\omega_{\mathbf{k}_1}}) \frac{b^{\parallel}}{2} [n_{\mathbf{k}}^{\uparrow/\downarrow} - n_{\mathbf{k}_1}^{\uparrow/\downarrow}] + \right. \\ \left. + \Re(G_{\omega_{\mathbf{k}}}^{\omega_{\mathbf{k}_1} \pm \omega_M}) [b^{\pm} n_{\mathbf{k}}^{\downarrow/\uparrow} - b^{\mp} n_{\mathbf{k}_1}^{\uparrow/\downarrow} \mp 2b^0 n_{\mathbf{k}_1}^{\uparrow/\downarrow} n_{\mathbf{k}}^{\downarrow/\uparrow}] \right\} \end{aligned} \quad (7a)$$

$$\begin{aligned} \frac{\partial}{\partial t} \mathbf{s}_{\mathbf{k}_1}^{\perp} = - \sum_{\mathbf{k}} \left[\Re(G_{\omega_{\mathbf{k}}}^{\omega_{\mathbf{k}_1} - \omega_M}) \left(\frac{b^+}{2} - b^0 n_{\mathbf{k}}^{\uparrow} \right) \mathbf{s}_{\mathbf{k}_1}^{\perp} + \right. \\ \left. + \Re(G_{\omega_{\mathbf{k}}}^{\omega_{\mathbf{k}_1} + \omega_M}) \left(\frac{b^-}{2} + b^0 n_{\mathbf{k}}^{\downarrow} \right) \mathbf{s}_{\mathbf{k}_1}^{\perp} + \Re(G_{\omega_{\mathbf{k}}}^{\omega_{\mathbf{k}_1}}) \frac{b^{\parallel}}{2} (\mathbf{s}_{\mathbf{k}}^{\perp} + \mathbf{s}_{\mathbf{k}_1}^{\perp}) \right] + \\ + \frac{\langle \mathbf{S} \rangle}{|\langle \mathbf{S} \rangle|} \times \left[\omega_M - \sum_{\mathbf{k}} \left\{ \Im(G_{\omega_{\mathbf{k}}}^{\omega_{\mathbf{k}_1} - \omega_M}) \left(\frac{b^+}{2} - b^0 n_{\mathbf{k}}^{\uparrow} \right) + \right. \right. \\ \left. \left. - \Im(G_{\omega_{\mathbf{k}}}^{\omega_{\mathbf{k}_1} + \omega_M}) \left(\frac{b^-}{2} + b^0 n_{\mathbf{k}}^{\downarrow} \right) \right\} \right] \mathbf{s}_{\mathbf{k}_1}^{\perp}, \end{aligned} \quad (7b)$$

where in favor of a compact notation, the variables for the occupations and spins have been transformed into the occupations of the spin-up and spin-down band, i. e., the diagonal elements of the reduced electron density matrix, according to:

$$n_{\mathbf{k}_1}^{\uparrow/\downarrow} := \frac{n_{\mathbf{k}_1}}{2} \pm s_{\mathbf{k}_1}^{\parallel}. \quad (8)$$

The coefficients used in Eqs. (7) are given by $b^{\pm} := \langle S^{\perp 2} \rangle \pm \frac{\langle S^{\parallel} \rangle}{2}$, $b^0 := \frac{\langle S^{\parallel} \rangle}{2}$ as well as $b^{\parallel} := \langle S^{\parallel 2} \rangle$, where $S^{\parallel} := \hat{\mathbf{S}} \cdot \frac{\langle \hat{\mathbf{S}} \rangle}{|\langle \hat{\mathbf{S}} \rangle|}$ is the Mn spin operator component parallel to the average Mn spin and $\langle S^{\perp 2} \rangle = \frac{1}{2} \langle S^2 - S^{\parallel 2} \rangle$. The remaining integral together with some prefactors are subsumed into the memory function

$$G_{\omega_{\mathbf{k}}}^{\omega_{\mathbf{k}_1}} := \frac{J_{sd}^2}{\hbar^2} \frac{n_{Mn}}{V} \int_{-t}^0 dt' e^{i(\omega_{\mathbf{k}} - \omega_{\mathbf{k}_1})t'}. \quad (9)$$

Eqs. (7) together with the memory in Eq. (9) describe the spin dynamics of the conduction band electron, where the precession of the electron spins and electron-impurity correlations are accounted for and will henceforth be referred to as the PESC equations. Note that to account for finite memory effects, the memory $G_{\omega_{\mathbf{k}}}^{\omega_{\mathbf{k}_1}}$ has to be regarded as an integral operator and the spins and occupations in the r.h.s. of Eqs. (7) have to be evaluated at the time $t + t'$.

3. Results and Discussion

3.1. Markov Limit of Effective Equations

The Eqs. (7) are written in terms of dynamical variables that depend on the \mathbf{k} -vector including the angles. This is important for possible extensions of the theory with \mathbf{k} -dependent effective magnetic fields resulting from, e. g., Dresselhaus[28]- and

Rashba[29]-terms. Without such extensions, angle-averaged equations can be obtained after going over to the Markov limit from which the physical meaning of the individual terms in the PESC Eqs. (7) will become most obvious. Technically, this is done by letting the lower integral bound $-t$ go to $-\infty$ in the memory function $G_{\omega_{\mathbf{k}}}^{\omega_{\mathbf{k}_1}}$. The memory is then given by:

$$G_{\omega_{\mathbf{k}}}^{\omega_{\mathbf{k}_1}} \approx \frac{J_{sd}^2}{\hbar^2} \frac{n_{Mn}}{V} \left\{ \pi \delta(\omega_{\mathbf{k}} - \omega_{\mathbf{k}_1}) - \mathcal{P} \frac{i}{\omega_{\mathbf{k}} - \omega_{\mathbf{k}_1}} \right\}. \quad (10)$$

The memory $G_{\omega_{\mathbf{k}}}^{\omega_{\mathbf{k}_1}}$ contains a Dirac delta distribution with respect to the frequencies $\omega_{\mathbf{k}}$. This allows us to derive from the PESC Eqs. (7) closed equations for dynamical variables that depend only on the frequencies. To this end, we define the following averaged quantities:

$$n_{\omega_1}^{\uparrow/\downarrow} := \frac{\sum_{\mathbf{k}} n_{\mathbf{k}}^{\uparrow/\downarrow} \delta(\omega_{\mathbf{k}} - \omega_1)}{\sum_{\mathbf{k}} \delta(\omega_{\mathbf{k}} - \omega_1)} \quad (11a)$$

$$\mathbf{s}_{\omega_1}^{\perp} := \frac{\sum_{\mathbf{k}} \mathbf{s}_{\mathbf{k}}^{\perp} \delta(\omega_{\mathbf{k}} - \omega_1)}{\sum_{\mathbf{k}} \delta(\omega_{\mathbf{k}} - \omega_1)}. \quad (11b)$$

Due to the delta distribution in Eq. (10), it becomes clear that the first term in Eq. (7a) for the spin-up and spin-down occupations disappears. Therefore, performing the Markov limit of Eqs. (7) and averaging over the angles, we obtain the following equations for the averaged variables $n_{\omega_1}^{\uparrow/\downarrow}$ and $s_{\omega_1}^{\perp} := |\mathbf{s}_{\omega_1}^{\perp}|$:

$$\frac{\partial}{\partial t} n_{\omega_1}^{\uparrow} = cD(\omega_2) \left\{ b^+ n_{\omega_2}^{\downarrow} - b^- n_{\omega_1}^{\uparrow} - 2b^0 n_{\omega_1}^{\uparrow} n_{\omega_2}^{\downarrow} \right\} \quad (12a)$$

$$\frac{\partial}{\partial t} n_{\omega_2}^{\downarrow} = cD(\omega_1) \left\{ b^- n_{\omega_1}^{\uparrow} - b^+ n_{\omega_2}^{\downarrow} + 2b^0 n_{\omega_1}^{\uparrow} n_{\omega_2}^{\downarrow} \right\} \quad (12b)$$

$$\begin{aligned} \frac{\partial}{\partial t} s_{\omega_1}^{\perp} = & -c \left\{ (D(\omega_0) + D(\omega_2)) \frac{\langle S^{\perp 2} \rangle}{2} + D(\omega_1) \langle S^{\parallel 2} \rangle + \right. \\ & \left. - \frac{\langle S^{\parallel} \rangle}{2} (D(\omega_0) n_{\omega_0}^{\uparrow} - D(\omega_2) n_{\omega_2}^{\downarrow}) \right\} s_{\omega_1}^{\perp}, \end{aligned} \quad (12c)$$

where $\omega_0 := \omega_1 - \omega_M$ and $\omega_2 := \omega_1 + \omega_M$. Here, we have used that in the quasi-continuum limit $\sum_{\mathbf{k}} \rightarrow \int d\omega D(\omega)$ with $D(\omega)$ being the density of states (DOS), and thus:

$$\sum_{\mathbf{k}} \Re(G_{\omega_{\mathbf{k}}}^{\omega_{\mathbf{k}_1}}) = \frac{J_{sd}^2}{\hbar^2} \frac{n_{Mn}}{V} \pi \sum_{\mathbf{k}} \delta(\omega_{\mathbf{k}} - \omega_{\mathbf{k}_1}) = \underbrace{\frac{J_{sd}^2}{\hbar^2} \frac{n_{Mn}}{V} \pi}_{=:c} D(\omega_1). \quad (13)$$

Therefore, it can be seen from Eqs. (12a-b) that in the Markov limit of the PESC equations, the only dynamical variables entering the equation of motion for the spin-up electrons $n_{\omega_1}^{\uparrow}$ with frequency ω_1 are $n_{\omega_2}^{\downarrow}$ and $n_{\omega_1}^{\uparrow}$ itself. Equally, the time evolution of $n_{\omega_2}^{\downarrow}$ only depends on $n_{\omega_1}^{\uparrow}$ and $n_{\omega_2}^{\downarrow}$, so that this pair of occupations is completely decoupled from the rest of the dynamical variables. Furthermore, the total number of electrons in the pair of occupations $n_{\omega_1}^{\uparrow}$ and $n_{\omega_2}^{\downarrow}$ is conserved, since from Eqs. (12a-b) it follows:

$$\frac{\partial}{\partial t} z_{\omega_1} = 0, \quad (14a)$$

where

$$z_{\omega_1} := D(\omega_1) n_{\omega_1}^{\uparrow} + D(\omega_2) n_{\omega_2}^{\downarrow}. \quad (14b)$$

Eq. (14a) allows us to merge Eqs. (12a-b) into a one-dimensional differential equation:

$$\begin{aligned} \frac{\partial}{\partial t} x_{\omega_1} = & 2cb^0 x_{\omega_1}^2 - c[D(\omega_1)b^+ + D(\omega_2)b^- + 2b^0 z_{\omega_1}]x_{\omega_1} \\ & + cD(\omega_1)b^+ z_{\omega_1} \end{aligned} \quad (15)$$

for the spectral electron density in the spin-up subband $x_{\omega_1} := D(\omega_1)n_{\omega_1}^\uparrow$.

The last term in Eq. (12a) and (12b), respectively, is a consequence of the source terms $b_{\beta\mathbf{k}_1}^{\alpha\mathbf{k}_2 I.2}$ in Ref. [26] which were associated with Pauli blocking in the golden rule-type rate equations that did not account for the precession of the correlations. This fact is also visible here, since for $n_{\omega_1}^\uparrow \approx 1$, Eq. (12a) yields

$$\frac{\partial}{\partial t} n_{\omega_1}^\uparrow = cD(\omega_2)(\langle S^{\perp 2} \rangle - \frac{\langle S^\parallel \rangle}{2})(n_{\omega_2}^\downarrow - 1), \quad (16a)$$

while without the last term of Eq. (12a), the limit would be

$$\frac{\partial}{\partial t} n_{\omega_1}^\uparrow = cD(\omega_2)(\langle S^{\perp 2} \rangle (n_{\omega_2}^\downarrow - 1) + \frac{\langle S^\parallel \rangle}{2}(n_{\omega_2}^\downarrow + 1)) \quad (16b)$$

Since the minimal value of $\langle S^{\perp 2} \rangle$ is $\frac{35}{12}$ which is greater than the maximal value of $\frac{\langle S^\parallel \rangle}{2}$ of $\frac{5}{4}$, the r.h.s. of Eq. (16a) is always non-positive, so an over-occupation of $n_{\omega_1}^\uparrow$ with values greater than 1 is averted. In contrast, in Eq. (16b) the occupation $n_{\omega_1}^\uparrow$ can exceed the physically reasonable limit of 1, e. g., in the case $n_{\omega_2}^\downarrow \approx 1$. Thus, again, the terms resulting from $b_{\beta\mathbf{k}_1}^{\alpha\mathbf{k}_2 I.2}$ in Ref. [26] are shown to provide for Pauli blocking effects.

The equation of motion (12c) for the electron spin component perpendicular to the Mn magnetization suggest an almost exponential decay to zero, but the occupations of the spin-up electrons at $\omega_1 - \omega_M$ and spin-down electrons at $\omega_1 + \omega_M$ enter in the effective decay rate. The appearance of the occupations is also due to the $b_{\beta\mathbf{k}_1}^{\alpha\mathbf{k}_2 I.2}$ terms. Here, they do not represent Pauli blocking, but are a remnant of the Landau-Lifshitz-Gilbert-like damping term structure in the Markov limit in Ref. [26], since:

$$\frac{\langle S^\parallel \rangle}{2}(D(\omega_0)n_{\omega_0}^\uparrow - D(\omega_2)n_{\omega_2}^\downarrow)s_{\mathbf{k}_1}^\perp = \frac{\langle S^\parallel \rangle}{2}\left(\frac{z_{\omega_0} - z_{\omega_1}}{2} + s_{\omega_1}^\parallel\right)s_{\mathbf{k}_1}^\perp \quad (17)$$

and

$$\left[\mathbf{s}_\omega \times (\mathbf{s}_{\omega_1} \times \langle \mathbf{S} \rangle) \right]_\perp = \langle S^\parallel \rangle s_\omega^\parallel s_{\omega_1}^\perp. \quad (18)$$

In fact, comparing the derivation of the Markov limit with and without accounting for the precession of the correlations it can easily be seen that the PESC Markov Eqs. (12) lead to the Markov Eq. (10) of Ref. [26], when ω_M is set to zero in the memory terms $G_{\omega_1 \pm \omega_M}^{\omega_1 \pm \omega_M}$.

3.2. Analytical solutions

The Markov limit of the PESC equations allows us to find analytic solutions which we will derive in the following.

3.2.1. *without Pauli blocking* If the terms resulting from $b_{\beta\mathbf{k}_1}^{\alpha\mathbf{k}_2 I.2}$ are neglected, Eqs. (12a) and (12b) yield:

$$\frac{\partial}{\partial t}x_{\omega_1} = -c(D(\omega_1)b^+ + D(\omega_2)b^-)x_{\omega_1} + cD(\omega_1)b^+z_{\omega_1}. \quad (19)$$

The solution of Eq. (19) decays exponentially:

$$x_{\omega_1}(t) = (x_{\omega_1}(0) - \xi_{\omega_1})e^{-\eta_{\omega_1}t} + \xi_{\omega_1}, \quad (20a)$$

with

$$\eta_{\omega_1} := c(D(\omega_1)b^+ + D(\omega_2)b^-) \quad (20b)$$

$$\xi_{\omega_1} := \frac{D(\omega_1)b^+}{D(\omega_1)b^+ + D(\omega_2)b^-}z_{\omega_1} \quad (20c)$$

It should be noted that for $D(\omega_2) \rightarrow D(\omega_1)$, the rate η_{ω_1} reaches the same value as for the rate equations of Ref. [26] and Fermi's golden rule[1, 25] when only the parabolic band energy is accounted for the initial and final states. Here, η_{ω_1} describes rates that can be derived with Fermi's golden rule, when the mean field energy difference between electrons in the spin-up and spin-down subbands $\hbar\omega_M$ is substituted into the band structure and transitions between these now non-degenerate subbands are considered.

Furthermore, without the terms originating from $b_{\beta\mathbf{k}_1}^{\alpha\mathbf{k}_2 I.2}$, the perpendicular component of the electron spin changes according to

$$\frac{\partial}{\partial t}s_{\omega_1}^\perp = - \underbrace{c \left\{ (D(\omega_0) + D(\omega_2)) \frac{\langle S^{\perp 2} \rangle}{2} + D(\omega_1) \langle S^{\parallel 2} \rangle \right\}}_{\gamma_{\omega_1}^\perp :=} s_{\omega_1}^\perp \quad (21)$$

which is solved by

$$s_{\omega_1}^\perp(t) = s_{\omega_1}^\perp(0)e^{-\gamma_{\omega_1}^\perp t} \quad (22)$$

It should be noted that neglecting the $b_{\beta\mathbf{k}_1}^{\alpha\mathbf{k}_2 I.2}$ terms in the rate equations without accounting for the precession of the correlations yielded the same expression for the rate that can also be obtained by letting $D(\omega_0)$ and $D(\omega_2)$ go to $D(\omega_1)$ in Eq. (21). In Ref. [26] it was found that including the precession of the correlation in the calculation did not significantly change the spin dynamics of the perpendicular component. Now, this can be understood by Taylor-expanding the DOS. Since in three dimensions, the DOS is proportional to the square root of ω , we find:

$$D(\omega_1 \pm \omega_M) = D(\omega_1) \sqrt{1 \pm \frac{\omega_M}{\omega_1}} \quad (23a)$$

and therefore

$$D(\omega_0) + D(\omega_2) = 2D(\omega_1) + \mathcal{O} \left(\left(\frac{\omega_M}{\omega_1} \right)^2 \right). \quad (23b)$$

Since the difference between the rates for the perpendicular component with and without accounting for the precession of the correlations is of second order of the ratio $\frac{\omega_M}{\omega_1}$, significant deviations can only be expected for small values of ω_1 . There, however, the DOS is rather small.

3.2.2. with Pauli blocking Eq. (15) is a Riccati differential equation with constant coefficients. Also in the case of golden rule-type rate equations derived from the original quantum kinetic theory, where the precession of the correlations around the Mn magnetization is neglected, we found an equation for the parallel electron spin component of this form[26]. The solutions of Eq. (15) can be obtained along the line of the Appendix in Ref. [26]:

$$x_{\omega_1}(t) = \frac{\mu_{\omega_1}}{2cb^0} - \frac{\nu_{\omega_1}}{2cb^0} \tanh\left(\frac{\varphi_{\omega_1}}{2} + \nu_{\omega_1}t\right), \quad (24a)$$

with

$$\mu_{\omega_1} = \frac{c}{2} [D(\omega_1)b^+ + D(\omega_2)b^- + 2b^0z_{\omega_1}], \quad (24b)$$

$$\nu_{\omega_1} = \sqrt{\mu^2 - 2c^2D(\omega_1)b^+b^0z_{\omega_1}}, \quad (24c)$$

where z_{ω_1} and φ_{ω_1} are determined by the initial values of $n_{\omega_1}^\uparrow$ and $n_{\omega_2}^\downarrow$.

Finally, the time dependence of the perpendicular spin component can be calculated using the analytical expressions for $n_{\omega_0}^\uparrow$ and $n_{\omega_2}^\downarrow$ and reads:

$$s_{\omega_1}^\perp(t) = s_{\omega_1}^\perp(0)e^{-\gamma_{\omega_1}^\perp t} e^{-b^0c \int_0^t dt' (D(\omega_0)n_{\omega_0}^\uparrow(t') - D(\omega_2)n_{\omega_2}^\downarrow(t'))} \quad (25)$$

In order to explicitly give the corresponding analytical expressions we have to distinguish two cases:

For $\omega_1 < \omega_M$, $D(\omega_0)$ vanishes and we find from Eq. (25):

$$s_{\omega_1}^\perp(t) = s_{\omega_1}^\perp(0)e^{-\gamma_{\omega_1}^\perp t} e^{(b^0cz_{\omega_1} - \frac{1}{2}\mu_{\omega_1})t} \sqrt{\frac{\cosh(\frac{\varphi_{\omega_1}}{2} + \nu_{\omega_1}t)}{\cosh(\frac{\varphi_{\omega_1}}{2})}}, \quad (26a)$$

and for $\omega_1 > \omega_M$ we obtain:

$$s_{\omega_1}^\perp(t) = s_{\omega_1}^\perp(0)e^{-\gamma_{\omega_1}^\perp t} e^{(b^0cz_{\omega_1} - \frac{1}{2}\mu_{\omega_0} - \frac{1}{2}\mu_{\omega_1})t} \times \\ \times \sqrt{\frac{\cosh(\frac{\varphi_{\omega_1}}{2} + \nu_{\omega_1}t)}{\cosh(\frac{\varphi_{\omega_1}}{2})}} \sqrt{\frac{\cosh(\frac{\varphi_{\omega_0}}{2} + \nu_{\omega_0}t)}{\cosh(\frac{\varphi_{\omega_0}}{2})}}. \quad (26b)$$

3.3. Numerical studies

The validity of the approximations used to derive the Markov limit PESCs Eqs. (12) is now checked by comparing the predicted spin dynamics with the results of the full quantum kinetic theory of Ref. [20] including also the residual terms that are denoted as $b_{\beta\mathbf{k}_1}^{\alpha\mathbf{k}_2 Res}$ in Eq. (4c). We modeled a bulk DMS of $\text{Zn}_{0.93}\text{Mn}_{0.07}\text{Se}$ with the following parameters: the Kondo coupling constant $J_{sd} = 12 \text{ meVnm}^3$, the effective mass $m_e = 0.21 m_0$ and an initial average Mn spin of $\frac{1}{2}\hbar$ along the z-axis. The difference between the different levels of theory, especially the role of the Pauli blocking terms, can be particularly highlighted by choosing initial non-equilibrium conditions, where the initial electron occupations are modeled by step functions (cf. Fig. 1). [‡]

In a first calculation, the spin-up subband occupation was initially a step function with a cut-off energy at $\mu = 3 \text{ meV}$ for electrons in the spin-up subband, while the

[‡] If the Pauli blocking terms are neglected, the equations are linear in $\mathbf{s}_{\mathbf{k}}$ and $n_{\mathbf{k}}$. Therefore, the solutions of the equations for other initial occupations can be written as linear combinations of the solutions for the step functions.

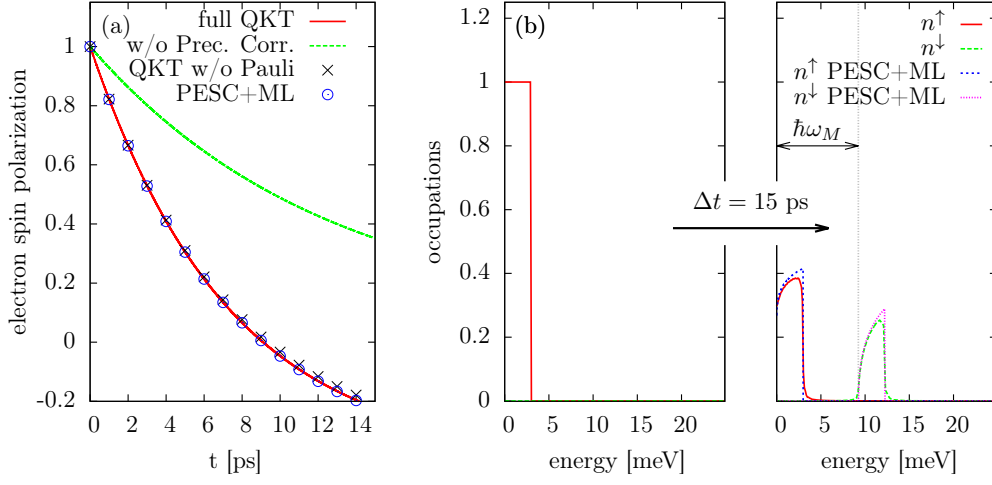


Figure 1. (a): Time evolution of the electron spin polarization of an initially step-like electron occupation in the spin-up subband. The red solid line is the result of a calculation using the full quantum kinetic theory (QKT) (cf. Ref. ([20])). The green dashed line is derived from the rate equations without taking the precession of the correlations (w/o Prec. Corr.) into account (cf. Ref. ([26])). The black crosses represent calculations of the quantum kinetic theory where the Pauli blocking terms $b_{\beta\mathbf{k}_2}^{\alpha\mathbf{k}_1 I.2}$ are neglected. The blue circles describe the spin dynamics according to the Markov limit of the PESC Eqs. (12). (b): Electron distributions at times $t = 0$ ps and $t = 15$ ps calculated using the full quantum kinetic theory and the Markov limit PESC equations, respectively.

spin-down subband was totally unoccupied for $t = 0$. The results are shown in Fig. 1 (a) where we plot the modulus of the total spin polarization

$$\mathbf{s}_{tot} = \left(\sum_{\mathbf{k}} \mathbf{s}_{\mathbf{k}} \right) \left(\sum_{\mathbf{k}} \frac{1}{2} n_{\mathbf{k}} \right)^{-1}. \quad (27)$$

There, the spin polarization is shown to decrease almost exponentially from the initially completely polarized configuration to a negative value according to the full quantum kinetic theory. While the calculation without accounting for the precession of the correlations deviates from the full quantum kinetic theory significantly, as it was already found in Ref. [26], the Markov limit of the PESC equations is able to reproduce the results of the full quantum kinetic theory almost perfectly. By comparison with the calculation neglecting the source terms $b_{\beta\mathbf{k}_2}^{\alpha\mathbf{k}_1 I.2}$ it can be seen that for the initial values used in this calculation, Pauli blocking effects are of minor importance.

Fig. 1 (b) depicts the energetic redistribution of the electrons: The initial step-like spin-up occupation evolves into a structure with two peaks; one in the spin-down and one in the spin-up band. The spin-up electrons with energy $\hbar\omega_1$ are redistributed to states with energy $\hbar\omega_1 + \hbar\omega_M$ which is predicted by the Markov limit of the PESC Eqs. (7) due to terms proportional to $\delta(\omega_{\mathbf{k}} - (\omega_{\mathbf{k}_1} \pm \omega_M))$. In contrast, when the precession of the correlations are neglected, the spin-down peak builds up at the same energetic position as the spin-up peak as the shift by $\hbar\omega_M$, which accounts for the precession-like dynamics of the Mn-carrier correlations, is missing in the delta distribution. The skewness of the peaks in Fig. 1 (b) arises from the square-root dependence of the DOS on the energy in a three dimensional system. The fact that a

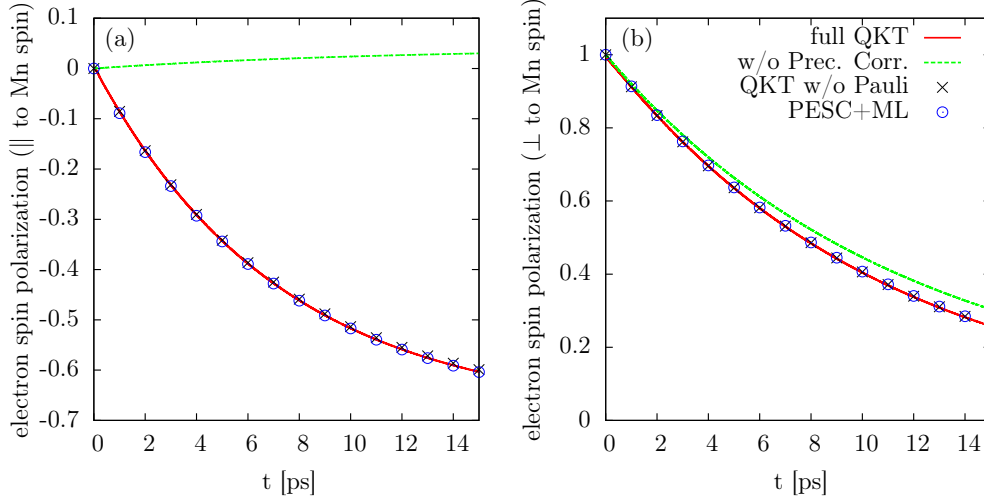


Figure 2. Time evolution of the spin polarization parallel (a) and perpendicular (b) to the Mn magnetization. The initial electron distribution is the same as in Fig. 1, except that the Mn magnetization was rotated 90° into a direction perpendicular to the initial electron spin (key as in Fig. 1a).

small tail is found below the spin-down peak representing occupations of states with energies lower than $\hbar\omega_M$ as well as a build-up of a high energy tail of the spin-up peak demonstrate slight non-Markovian deviations from the Dirac delta-like memory in the Markov limit of Eq. (10). These effects are, however, too small to influence the time dependence of the total spin polarization significantly.

Fig. 2 displays the time evolution of the electron spin polarization for a situation where the initial conditions were chosen as in the calculations for Fig. 1, except that the average Mn spin is now turned 90° away from the electron spin. Unlike the case discussed before, the spin polarization vector \mathbf{s}_{tot} now has components parallel and perpendicular to the Mn magnetization. Fig. 2 (a) shows a build-up of the spin polarization parallel to the Mn magnetization according to the full quantum kinetic theory which coincides with the calculations in the Markov limit of the PESC equations and the simulations without accounting for Pauli blocking. As in the previous calculations, the solution of the golden rule-type rate equation of Ref. [26] deviates significantly from the other calculations, since the energetic redistribution of the electrons is neglected. The time evolution of the perpendicular electron spin shown in Fig. 2 (b), however, is almost the same in all of the above calculations which can be understood by considering Eqs. (23).

In the following, we want to discuss the effects of Pauli blocking. To this end, we study a case, where both subbands are initially partly occupied and where the spin dynamics is especially clear: We use initial conditions that describe a situation, where the spin polarization is expected to be nearly constant if Pauli blocking is taken into account. Then, if we calculate the spin dynamics while neglecting the terms responsible for Pauli blocking effects, we can attribute the non-constant behavior to these effects. If the Hamiltonian (1) is treated on the mean field level, the equilibrium occupations at $T = 0$ of the spin-down and spin-up subbands follow spin-split Fermi distributions, i. e., step-functions, whose cut-off energies, measured from the respective

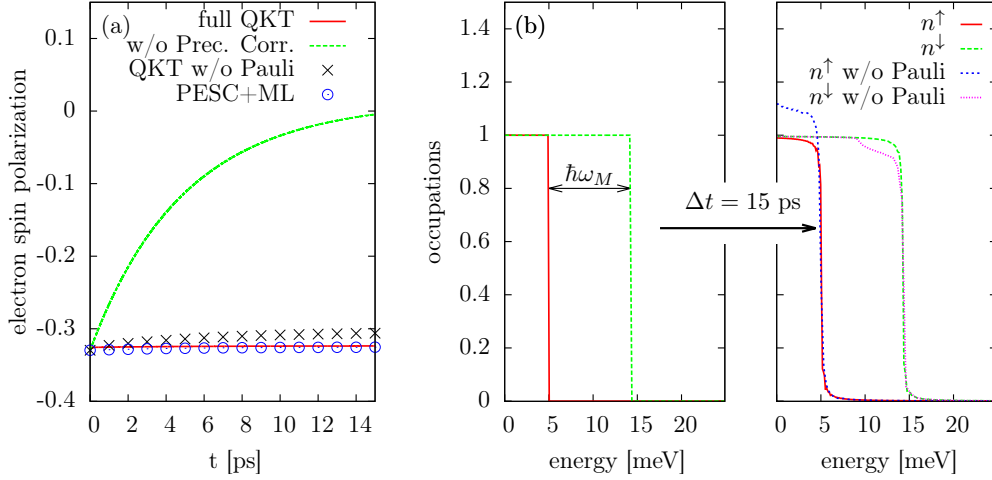


Figure 3. Time evolution of the spin polarization (a) and electron redistribution (b) of an initially step-like occupation of electrons where the difference of the cut-offs of the spin-up and spin-down subband occupations is $\hbar\omega_M$. In (b), the occupations are plotted for calculations based on the full quantum kinetic theory with and without the terms $b_{\beta\mathbf{k}_2}^{\alpha\mathbf{k}_1 I,2}$ accounting for Pauli blocking.

band edge, differ by $\hbar\omega_M$. The results of the calculations with these initial conditions are given in Fig. 3. Since the full quantum kinetic theory also accounts for the correlation energies, very small changes in the electron spin polarization are found, which are due to the build-up of correlations over the course of time. Fig. 3 (a) shows that the Markov limit of the PESc equations again yields nearly the same spin dynamics as the full quantum kinetic theory, while the rate equations without precession of the correlations fail to describe the spin polarization, since different states are coupled due to the neglect of ω_M in the Dirac delta function of the memory. The calculations involving the quantum kinetic theory without the Pauli blocking terms lead to surprisingly small deviations from the full quantum kinetic theory concerning the total spin polarization displayed in Fig. 3 (a), despite the unphysical build-up of occupations $n_\omega^\uparrow > 1$ for some values of ω seen in Fig. 3 (b). The electron occupations after $t = 15$ ps depicted in Fig. 3 (b) essentially follow the original step functions for the two spin orientations, but since the edges are smoothed due to the non-Markovian deviations from the delta distribution in the memory, they resemble Fermi distributions with a finite effective temperature.

4. Conclusion

We have derived effective equations of motion [cf. Eqs. (7)] for the conduction band electron spins and occupations starting from a microscopic quantum kinetic theory using a rotating-wave-like Ansatz. These equations account for the precession of the electron spins around the effective magnetic field due to the Mn magnetization as well as for a precession-like dynamics of the electron-Mn correlation functions. Therefore, in this article they are referred to as *precession of electron spins and correlations* (PESc) equations. The PESc equations can be more easily interpreted as the original quantum kinetic equations. They also provide an important speed-up

of the numerics, in particular, when the Markov limit of the PESC equations is used. The spin dynamics for high Mn doping in three dimensional systems derived from our effective equations in the Markov limit are demonstrated by numerical calculations to agree well with the corresponding results of the original quantum kinetic theory. This resolves the deficiency of the golden rule-type rate equations of Ref. [26] for the case of a finite initial impurity magnetization. Even though the PESC equations can in principle describe non-Markovian effects as well as Pauli blocking, the numerical studies suggest that these are of minor importance for the time evolution of the total electron spin polarization, at least for the situations studied in this paper.

The Markov limit of the PESC Eqs. (12) can be readily interpreted: For a positive coupling constant J_{sd} , spin-up electrons can gain energy in the mean field due to the Mn magnetization by a spin-flip process to the spin-down subband. Due to the total energy conservation, this energy is transformed into kinetic energy. Therefore, a spin-up state couples effectively only to a spin-down state with a kinetic energy $\hbar\omega_M$ greater than the spin-up state energy and vice-versa. The resulting equation can be solved analytically yielding a time dependence of the electron spin polarization following a tanh-function. If the Pauli blocking terms are neglected, the equations are solved by a simple decaying exponential function with a rate that can also be obtained by applying Fermi's golden rule, if the mean field energy of an electron in the effective field of the Mn magnetization is included into the single particle energies.

Numerical studies of the energetic redistribution of the electrons in the full quantum kinetic theory support the findings of the delta-like coupling of states in energy space in general, but slight deviations from this Markovian prediction can be seen especially in the smoothing of sharp edges of the initial electron occupations. It is expected that the non-Markovian features will be more important in two-dimensional systems[25, 30]. The PESC equations in the Markov limit derived in this paper can provide a suitable framework for further investigations of these effects. In addition, their numerical simplicity allows for the introduction of other mechanisms of spin relaxation to study reliably their competition with the s - d exchange interaction which would be a demanding task within the original quantum kinetic theory.

Acknowledgments

We acknowledge the support by the Deutsche Forschungsgemeinschaft through the Grant No. AX 17/9-1.

References

- [1] Kossut J 1975 *physica status solidi (b)* **72** 359–367
- [2] Furdyna J K 1988 *Journal of Applied Physics* **64** R29–R64
- [3] Krenn H, Kaltenegger K, Dietl T, Spalek J and Bauer G 1989 *Phys. Rev. B* **39**(15) 10918–10934
- [4] Crooker S A, Awschalom D D, Baumberg J J, Flack F and Samarth N 1997 *Phys. Rev. B* **56**(12) 7574–7588
- [5] Kikkawa J M and Awschalom D D 1998 *Phys. Rev. Lett.* **80**(19) 4313–4316
- [6] Akimov A V, Scherbakov A V, Yakovlev D R, Merkulov I A, Bayer M, Waag A and Molenkamp L W 2006 *Phys. Rev. B* **73**(16) 165328

- [7] Rönning K E, Mohler E, Roskos H G, Ortner K, Becker C R and Molenkamp L W 2006 *Phys. Rev. Lett.* **96**(11) 117203
- [8] Cywiński L and Sham L J 2007 *Phys. Rev. B* **76**(4) 045205
- [9] Jiang J H, Zhou Y, Korn T, Schüller C and Wu M W 2009 *Phys. Rev. B* **79**(15) 155201
- [10] Kapetanakis M D, Perakis I E, Wickey K J, Piermarocchi C and Wang J 2009 *Phys. Rev. Lett.* **103**(4) 047404
- [11] Wu M, Jiang J and Weng M 2010 *Phys. Rep.* **493** 61 – 236
- [12] Kossut J and Gaj J (eds) 2011 *Introduction to the Physics of Diluted Magnetic Semiconductors (Springer Series in Materials Science no 144)* (Berlin: Springer)
- [13] Camilleri C, Teppe F, Scalbert D, Semenov Y, Nawrocki M, Dyakonov M, Cibert J, Tatarenko S and Wojtowicz T 2001 *Phys. Rev. B* **64**(8) 085331
- [14] Myers R C, Mikkelsen M H, Tang J M, Gossard A C, Flatté M E and Awschalom D D 2008 *Nature Materials* **7** 203 – 208
- [15] Cronenberger S, Vladimirova M, Andreev S, Lifshits M and Scalbert D 2013 *Phys. Rev. Lett.* **110**(7) 077403
- [16] Chen W, Buyanova I, Rudko G, Mal'shukov A, Chao K, Toropov A, Terent'ev Y, Sorokin S, Lebedev A, Ivanov S and Kop'ev P 2003 *Phys. Rev. B* **67**(12) 125313
- [17] Smyth J, Tulchinsky D, Awschalom D, Samarth N, Luo H and Furdyna J 1993 *Phys. Rev. Lett.* **71**(4) 601–604
- [18] Chen Y, Wiater M, Karczewski G, Wojtowicz T and Bacher G 2013 *Phys. Rev. B* **87**(15) 155301
- [19] Ben Cheikh Z, Cronenberger S, Vladimirova M, Scalbert D, Perez F and Wojtowicz T 2013 *Phys. Rev. B* **88**(20) 201306
- [20] Thurn C and Axt V M 2012 *Phys. Rev. B* **85**(16) 165203
- [21] D'yakonov M I and Perel' V I 1971 *Zh. Eksp. Teor. Fiz.* **60** 1954 [Sov. Phys. JETP **33**, 1053 (1971)]
- [22] Yafet Y 1963 (*Solid State Physics* vol 14) (Academic Press, New York)
- [23] Elliott R J 1954 *Phys. Rev.* **96**(2) 266–279
- [24] Bir G L, Aronov A and Pikus G E 1975 *JETP* **42** 705
- [25] Thurn C, Cygorek M, Axt V M and Kuhn T 2013 *Phys. Rev. B* **87**(20) 205301
- [26] Cygorek M and Axt V M 2014 *Phys. Rev. B* **90**(3) 035206
- [27] Hilton D J and Tang C L 2002 *Phys. Rev. Lett.* **89**(14) 146601
- [28] Dresselhaus G 1955 *Phys. Rev.* **100**(2) 580–586
- [29] Bychkov Y A and Rashba E I 1984 *Journal of Physics C: Solid State Physics* **17** 6039
- [30] Thurn C, Cygorek M, Axt V M and Kuhn T 2013 *Phys. Rev. B* **88**(16) 161302(R)